Modifying Dihedral Angles

Protein molecules are formed by joining a series of amino acids into a chain. The order of the amino acids in this series is called the amino acid sequence of the molecule. All amino acids have a set of 6 atoms in common. These atoms form the "backbone" of the protein. The conformation (shape) of the protein can be described with 3 angles for each amino acid. Additional angles must be added for the orientations of the individual sidechains, but the 3 are responsible for defining the overall structure of the protein. Here is a (poor quality at the moment) diagram defining these angles. If you want to know more, read a book on protein chemistry. I would reccomend Principles of Protein Structure, by Schulz and Schirmer. This diagram is reproduced without permission from p.19 of that book (sorry for the low quality).

dihed.tiff ¬

In any case, MolViewer provides you with the ability to change these angles in proteins assembled with Alchemy. MolViewer uses Alchemy's notation of amide nitrogens to locate the individual amino acids, so ONLY proteins created with Alchemy will currently work.

One of the 3 angles, ω, is generally rigid at 180 degrees. For any realistic protein structure you need to leave it set to 180 (or equivalently -180). Depending on the amino acids in your protein, there are also

limitations on the allowable angles for ψ and ϕ. The two most common protein structures, α-helix and β-sheet are located near angles (-60,-60) and (120,-60) respectively. Again, read a protein chemistry book for more details.

A couple of the sample files I included are proteins you can play with. Hopefully in future versions you will be able to use PDB files directly without filtering through alchemy first.

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